

## COVER SHEET

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Title: **Order-Reduced Solution of the Nonlinear High-Fidelity Generalized Method of Cells Micromechanics Relations**

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## ABSTRACT

The High-Fidelity Generalized Method of Cells (HFGMC) is one technique for accurately simulating nonlinear composite material behavior. The HFGMC uses a higher-order approximation for the subcell displacement field that allows for a more accurate determination of the subcell stress/strain fields at the cost of some computational efficiency. In order to reduce computational costs associated with the solution of the ensuing system of simultaneous equations, the HFGMC global system of equations for doubly-periodic repeating unit cells with nonlinear constituents was reduced in size through the use of a Petrov-Galerkin-based Proper Orthogonal Decomposition order-reduction scheme. A number of cases were presented that address the computational feasibility of using order-reduction techniques to solve solid mechanics problems involving complex microstructures.

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## INTRODUCTION

The High-Fidelity Generalized Method of Cells (HFGMC) is a micromechanics technique that can be used to simulate nonlinear composite materials [1]. The core computational effort of this method involves repeatedly finding the solution to sets of simultaneous equations in order to establish effective properties and solve a boundary value problem of interest. However, when material nonlinearity is admitted, the computational runtimes can become excessive, particularly as the problem size is increased. Nonlinear analyses of higher-fidelity repeating unit cells (RUCs) are needed to accurately simulate realistic composite microstructures necessary for process modeling, prediction of residual stress states, progressive failure analysis, and other computational predictions that depend heavily on subscale features. The use of order-reduction techniques is one possibility to improve the computational efficiency of high-fidelity analyses.

A significant fraction of studies employ Proper Orthogonal Decomposition (POD) [2-3] to generate order-reduced models. POD is commonly used in the finite element community to reduce the dimensionality of a large set of simultaneous equations. The goal of POD in this context is to generate a set of basis functions capable of capturing the dominant components of a system. These basis functions are then used to optimally represent a full set of equations and provide a mapping relationship between the normal and reduced domains. POD-based order-reduction techniques have been previously used to solve nonlinear problems in computational micromechanics [4-7]. For instance, Radermacher *et al.* [4] was able to obtain a 60-260 computational speed-up by employing a POD-based order-reduction technique for an inelastic metal matrix composite.

In the present work, the HFGMC global system of equations for doubly-periodic RUCs with nonlinear constituents is reduced in size through the use of POD. This approach previously was shown to yield significant computational savings when applied to the HFGMC equations for linearly elastic materials only [8]. The order-reduced HFGMC models are then compared to the traditional HFGMC approach for multiple RUCs in order to assess their computational efficiency.

## HIGH-FIDELITY GENERALIZED METHOD OF CELLS (HFGMC)

The HFGMC is a micromechanics technique used for modeling heterogeneous materials [1]. In contrast to the generalized method of cells [1], the HFGMC gives a higher accuracy in the subcell stress/strain fields at the cost of computational efficiency by employing a higher-order subcell displacement field. Using the HFGMC, a doubly or triply periodic RUC is discretized into an arbitrary number of subcells (see Figure 1). A doubly-periodic RUC may be defined in the  $y_2$ - $y_3$  plane and is discretized into  $N_\beta$  and  $N_\gamma$  subcells along the  $y_2$ -direction (height) and the  $y_3$ -direction (width), respectively, while the inclusions (fibers) extend infinitely in the  $y_1$ -direction (length). A local  $\bar{y}_2^{(\beta)}$ - $\bar{y}_3^{(\gamma)}$  coordinate system may be defined relative to the centroid of each subcell. The height and length of each subcell are given by  $h_\beta$  and  $l_\gamma$ , respectively. The discussion that follows presents key aspects of the HFGMC formulation that are relevant to this study. An exhaustive derivation of the HFGMC can be found in Ref. [1].

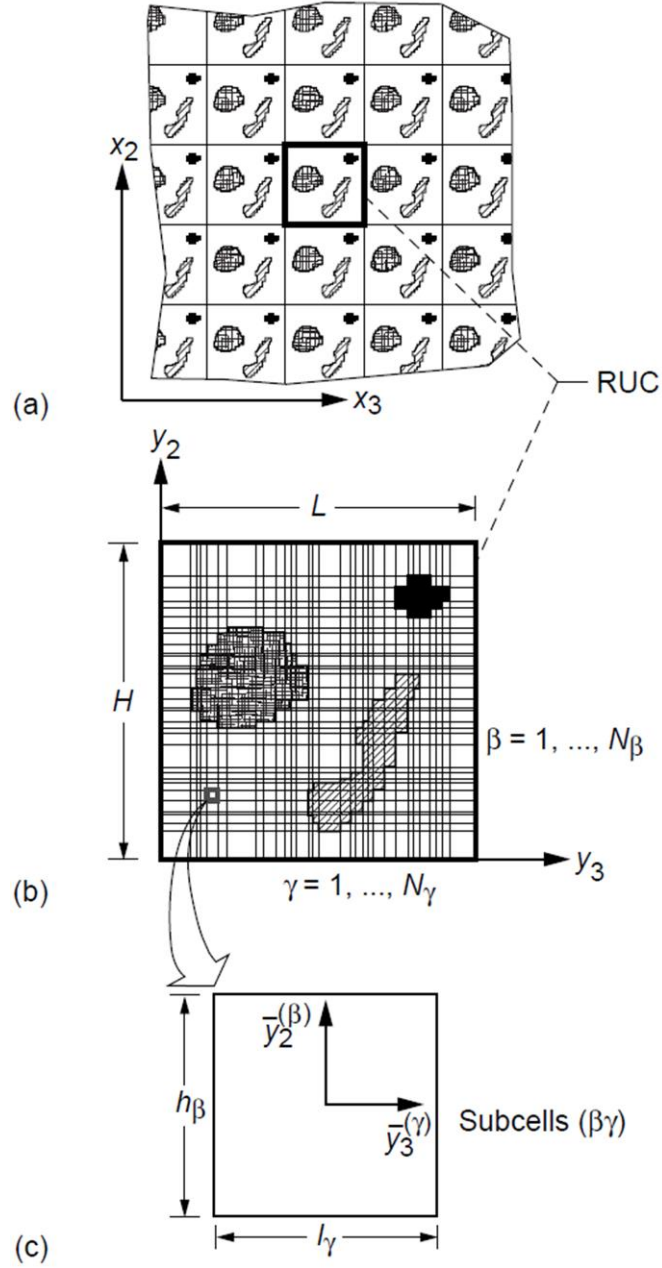


Figure 1. A heterogeneous composite with a doubly-periodic microstructure comprised of a) multiple repeating RUCs. b) A single RUC of dimensions  $H \times L$  comprised of a number of individual subcells. c) An individual subcell of dimensions  $h_\beta \times l_\gamma$ . Here,  $x_i$ ,  $y_i$ , and  $\bar{y}_i$  refer to global, RUC, and subcell coordinates, respectively ( $i = 1 \dots 3$ ). Figure from Ref. [1].

### HFGMC Subcell Equations

Each subcell in an RUC is assigned material properties and a constitutive law to describe the local material behavior. The constitutive law for thermoelastic materials is given by Eq. 1:

$$\sigma_{ij}^{(\beta\gamma)} = C_{ijkl}^{(\beta\gamma)} \left( \varepsilon_{kl}^{(\beta\gamma)} - \varepsilon_{kl}^{T^{(\beta\gamma)}} - \varepsilon_{kl}^{I^{(\beta\gamma)}} \right) \quad i, j, k, l = 1, 2, 3 \quad (1)$$

where  $\boldsymbol{\sigma}^{(\beta\gamma)}$ ,  $\boldsymbol{C}^{(\beta\gamma)}$ ,  $\boldsymbol{\varepsilon}^{T^{(\beta\gamma)}}$ , and  $\boldsymbol{\varepsilon}^{I^{(\beta\gamma)}}$  are the stress, stiffness, thermal strain, and inelastic strain tensors, respectively. The stress tensor is used to calculate surfaced-averaged tractions,  $\boldsymbol{t}^{(\beta\gamma)}$ , along the edges of a subcell as a function of the unknown fluctuating displacements. The computational efficiency of the HFGMC can be significantly improved by reformulating  $\boldsymbol{t}^{(\beta\gamma)}$  to be a function of *surface-averaged* fluctuating displacements (unknowns) [9-10]. A linear system of 12 equations can be derived and expressed as:

$$\boldsymbol{t}^{(\beta\gamma)} = \boldsymbol{K}^{(\beta\gamma)} \bar{\boldsymbol{u}}^{(\beta\gamma)} + \boldsymbol{f}^{(\beta\gamma)} + \boldsymbol{g}^{(\beta\gamma)} \quad (2)$$

where  $\bar{\boldsymbol{u}}^{(\beta\gamma)}$  represents the unknown surface-averaged fluctuating displacements,  $\boldsymbol{f}^{(\beta\gamma)}$  is a vector containing subcell material properties and macroscale strain components, and  $\boldsymbol{g}^{(\beta\gamma)}$  is a vector containing thermoinelastic components. The  $12 \times 12$  subcell stiffness matrix,  $\boldsymbol{K}^{(\beta\gamma)}$ , contains subcell material properties and dimensions and does not depend on any inelastic parameters.

### HFGMC Global Equations

By imposing interfacial traction and displacement continuity conditions, and periodic boundary conditions, an assembled, linear system of equations can be derived. For perfectly bonded constituents, the reformulated HFGMC relationships can be expressed as a square system of  $n = 6N_\beta N_\gamma$  equations of the form:

$$\boldsymbol{K}\boldsymbol{U} = \boldsymbol{f} + \boldsymbol{g} \quad (3)$$

where  $\boldsymbol{K}$  is a sparse, unsymmetrical matrix that is a function of subcell properties and geometry,  $\boldsymbol{f}$  is a vector containing the material properties/dimensions and the applied average strains, and  $\boldsymbol{g}$  is a vector containing material properties/dimensions and the thermoinelastic contribution. The vector  $\boldsymbol{U}$  represents the unknown surface-averaged fluctuating displacements for each subcell. These equations must be iteratively solved at each loading increment, and the solution is used to determine subcell stresses and strains. In the present HFGMC formulation, each row of  $\boldsymbol{K}$  effectively represents a traction continuity equation. The terms containing the unknown surface-averaged fluctuating displacements are collected on the left-hand side of Eq. 3, and all other terms are collected on the right-hand side. In general,  $\boldsymbol{K}$  must be assembled each time the constituent properties of a subcell change. Ongoing work is aimed at developing a direct assembly procedure similar to that for finite element problems [11-12] in order to only update components of  $\boldsymbol{K}$  that change.

### HFGMC Solution Procedure

In a typical HFGMC analysis, the assembled HFGMC system of  $n$  equations is solved multiple times, each with distinct boundary conditions and input parameters. In general, the equations are solved six times to establish the mechanical strain concentration tensor. This tensor is used to calculate the effective elastic stiffness and thermal stress tensors of the composite. The mechanical strain concentration tensor does not depend on the inelastic material state [1]. If all elastic material properties are

temperature independent, this step is only performed for the first loading increment (*i.e.*, the effective properties are constant). When thermoelastic/thermoelastic materials are considered, this step must be performed every increment where a temperature change occurs.

Additionally, for each loading increment, an iterative solution procedure is required to achieve converged inelastic fields. The Mendelson method [13-14] was used to integrate the classical plasticity equations at each integration point within a subcell. In the HFGMC, the global system of equations is solved two times *per iteration per increment*: once to solve the actual boundary value problem under consideration and another to update the inelastic field quantities for the next iteration/increment. Order-reduction techniques are hence an attractive option to reduce the computational cost associated with repeatedly assembling/solving the HFGMC system of equations.

## ORDER-REDUCTION CONCEPTS APPLIED TO THE HFGMC

### Proper Orthogonal Decomposition (POD)

As previously mentioned, POD is a technique that can be used to optimally represent a large system of equations. Suppose that the solution to Eq. 3 (*i.e.*,  $\mathbf{U}$  of length  $n$ ) can be obtained *a priori*. The vector  $\mathbf{U}$  can be expressed by  $\mathbf{U} = \mathbf{V}\mathbf{w}$  where  $\mathbf{V} = [\mathbf{V}_1, \mathbf{V}_2, \dots, \mathbf{V}_n]$  is a set of  $n$  arbitrary orthonormal basis vectors that span the solution space and  $\mathbf{w}$  is a coefficient vector of length  $n$ . The goal of POD is to determine an approximate solution to  $\mathbf{U}$ ,  $\hat{\mathbf{U}} = \hat{\mathbf{V}}\hat{\mathbf{w}}$  where  $\hat{\mathbf{V}} = [\mathbf{V}_1, \mathbf{V}_2, \dots, \mathbf{V}_k]$  is a set of the first  $k$  vectors of  $\mathbf{V}$ ,  $\hat{\mathbf{w}}$  is a vector comprised of the first  $k$  components of  $\mathbf{w}$ , and  $k \leq n$ . Note that for optimal computational performance,  $k \ll n$ .

The method of snapshots [15] was used to determine the set of  $k$  orthonormal basis vectors and, hence, the size of the reduced set of equations. Suppose that the solution to Eq. 3 (*i.e.*,  $\mathbf{U}$ ) for an RUC under a particular set of applied strains/stresses is known at a given increment (or iteration). This solution (*i.e.*, a “snapshot”) can be assigned to the first column of a new matrix,  $\mathbf{M}$ . Additional columns of  $\mathbf{M}$  can be populated using *any* converged (or pre-converged) incremental solutions to Eq. 3 for a given RUC architecture. A singular value decomposition (SVD) of the snapshot matrix,  $\mathbf{M}$ , can be performed and is expressed as:

$$\mathbf{M} = \mathbf{V}\mathbf{\Sigma}\mathbf{Z}^T \quad (4)$$

where  $\mathbf{V}$  and  $\mathbf{Z}$  are the left- and right-singular vectors, respectively, and  $\mathbf{\Sigma}$  is a diagonal matrix of singular values arranged in descending order. The matrix  $\mathbf{V}$  is then used to populate  $\hat{\mathbf{V}}$  [2].

### Order-reduced HFGMC

Consider the HFGMC system of equations given by Eq. 3 (referred to herein as the reference solution). As a result of performing POD, an approximate solution for  $\mathbf{U}$  can be expressed by  $\hat{\mathbf{U}} = \hat{\mathbf{V}}\hat{\mathbf{w}}$  where  $\hat{\mathbf{w}}$  can be referred to as the order-reduced solution vector. This approximate solution is substituted into Eq. 3 and results in an

overdetermined system of linear equations ( $n$  equations with  $k$  unknowns,  $k < n$ ) and a residual,  $\mathbf{r}$ .

$$\mathbf{K}\hat{\mathbf{V}}\hat{\mathbf{w}} = \mathbf{f} + \mathbf{g} + \mathbf{r} \quad (5)$$

The residual effectively contains contributions that fall outside of the subspace spanned by  $\hat{\mathbf{V}}$ . This implies that  $\hat{\mathbf{V}}^T \mathbf{r} = \mathbf{0}$  since each basis vector in  $\hat{\mathbf{V}}$  is orthogonal to  $\mathbf{r}$  (i.e., the contribution from the remaining basis vectors in  $\mathbf{V}$ ). The residual can be eliminated from Eq. 5 by multiplying each side by  $\hat{\mathbf{V}}^T$ . This imposes the orthogonality constraints on the residual and results in a reduced set of  $k \times k$  equations.

$$\hat{\mathbf{V}}^T \mathbf{K} \hat{\mathbf{V}} \hat{\mathbf{w}} = \hat{\mathbf{V}}^T (\mathbf{f} + \mathbf{g}) \quad (6)$$

In effect, the same basis vectors are used both for approximating the reference solution and performing the projection to the reduced system. This is commonly referred to as Galerkin-based POD. However, for nonlinear problems, a Galerkin projection method can lead to numerical instabilities, and a Petrov-Galerkin projection can be used to overcome these instabilities [16]. Rather than performing the projection by multiplying Eq. 5 by  $\hat{\mathbf{V}}^T$ , it can be multiplied by  $\hat{\mathbf{V}}^T \mathbf{K}^T$  resulting in a reduced set of  $k \times k$  equations.

$$\hat{\mathbf{V}}^T \mathbf{K}^T \mathbf{K} \hat{\mathbf{V}} \hat{\mathbf{w}} = \hat{\mathbf{V}}^T \mathbf{K}^T (\mathbf{f} + \mathbf{g}) \quad (7)$$

It should be noted that in order to set up the reduced set of equations, the  $n \times n$  matrix  $\mathbf{K}$  and  $n \times 1$  vectors  $\mathbf{f}$  and  $\mathbf{g}$  must be determined. The  $k \times k$  reduced stiffness matrix,  $\hat{\mathbf{K}} = \hat{\mathbf{V}}^T \mathbf{K}^T \mathbf{K} \hat{\mathbf{V}}$ , will only change if subcell properties are updated (e.g., due to a temperature change, damage, etc.). The approximate reference solution can be recovered by using the relationship  $\hat{\mathbf{U}} = \hat{\mathbf{V}} \hat{\mathbf{w}}$  once Eq. 7 is solved. In effect, the original set of  $n = 6N_\beta N_\gamma$  equations can be converted into a potentially much smaller set of  $k$  equations and solved. However, by only including  $k$  of the  $n$  orthonormal basis vectors, an error is introduced. The goal of an order-reduction technique in this context is to determine the smallest system of equations while minimizing the approximation error. An accurate reduced model can likely be generated provided that the orthonormal basis vectors capture the variation in input parameters.

## MICROSCALE SIMULATIONS OF THERMOINELASTIC COMPOSITES

### Analysis Details

The computational efficiency of the order-reduced HFGMC method was evaluated for an E-glass fiber and Nylon 12 matrix composite system. The E-glass fiber was assumed to be isotropic and linear elastic and was assigned temperature-independent material properties [17]. The Nylon 12 matrix was assumed to be isotropic with an elastic-perfectly plastic material response and temperature-dependent material properties [18-19]. The applicable Young's moduli ( $E$ ), Poisson's ratios ( $\nu$ ), secant coefficient of thermal expansions (CTE), and yield stresses ( $\sigma_y$ ) are presented in Table I as a function of temperature ( $T$ ).

TABLE I. FIBER AND MATRIX CONSTITUENT PROPERTIES

	$T$ (°C)	$E$ (MPa)	$\nu$	$\sigma_y$ (MPa)	CTE ( $\mu\text{s}/^\circ\text{C}$ )
Fiber	-	74000	0.20	-	4.9
Matrix	-25	2100	0.36	54.0	158.0
	0	1400	0.36	43.9	158.0
	23	950	0.36	28.0	158.0
	50	480	0.36	18.0	158.0

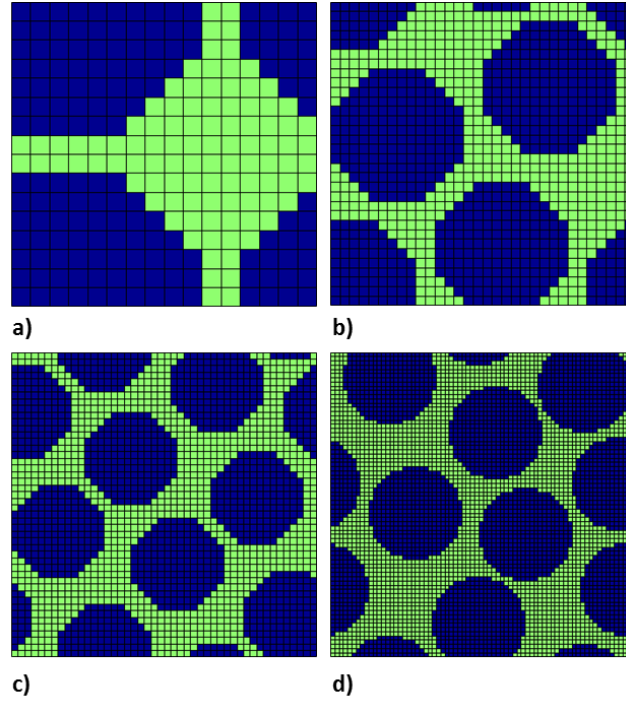


Figure 2. Four different randomized RUC architectures comprised of a) 256, b) 1024, c) 2116, and d) 5184 subcells where blue indicates a fiber subcell and green indicates a matrix subcell.

Ricks *et al.* [8] previously demonstrated that the computational efficiency of the order-reduced HFGMC for linearly elastic constituents significantly depends on the number of subcells in the RUC. In this study, four distinct RUCs with a nominal 60% fiber volume fraction and a random microstructure were generated using a recently developed RUC generator [20]. These RUCs have 256, 1024, 2116, and 5184 subcells and are shown in Figures 2 a-d, respectively.

In the HFGMC, a combination of global stress or strain components and temperature can be applied to an RUC. For this study, a 2% normal strain in the  $x_2$ -direction was applied over 150 loading increments to each of the four RUCs in Figure 2. With the exception of the axial stress in the  $x_2$ -direction, all other stress components were set to zero. Additionally, a linear temperature increase from  $-25^\circ\text{C}$  to  $50^\circ\text{C}$  was applied. The temperature and mechanical loads were imposed simultaneously in order to assemble and solve the HFGMC equations the maximum amount of times within a loading increment. Seven integration points per direction were assigned to each subcell. This number was found to be the minimum necessary to achieve convergence of the inelastic strain/stress field. A conservative number of

iterations (*i.e.*, 50) were performed for each increment. Since multiple unique RUCs were considered in this study, no robust criterion was specified to establish convergence of the inelastic fields. Rather, preliminary analyses were performed to determine the appropriate number of iterations necessary for convergence for all RUCs. By basing convergence on a fixed number of iterations, an appropriate comparison of the computational cost for the different RUCs can be performed without having to consider whether less/more iterations were required for a particular RUC analysis.

### **Generation of the Order-Reduced HFGMC Models**

As previously mentioned, the method of snapshots was used to determine the orthonormal basis vectors required to approximate the reference solution and project to the reduced subspace. This technique requires that the solution to each of HFGMC system of equations be obtained at a number of time/loading intervals. These basis vectors are substituted into Eq. 7 and used to generate an order-reduced model. This process was performed offline prior to performing an analysis of interest. For linearly elastic materials without any temperature change, the effective elastic stiffness tensor was calculated when generating the snapshots. This tensor can be stored and used to eliminate the need to calculate the mechanical strain concentration tensor in the order-reduced HFGMC. Additionally, since no inelasticity is permitted when considering only linearly elastic materials, this practically implies that the HFGMC system of equations is only required to be solved once per increment (no need for an iterative procedure). As such, Ricks *et al.* [8] demonstrated that a single order-reduced model can accurately and efficiently represent the full HFGMC system of equations.

However, when thermoinelastic materials are considered, multiple unique HFGMC systems of equations must be repeatedly assembled and solved. Preliminary analysis results indicated that a single order-reduced model should not be used for all eight unique sets of equations (*i.e.*, it was not accurate and computationally efficient). As such, separate, smaller models were generated for each set of equations. In order to establish the eight order-reduced models, the converged solution at each of 150 increments for each set of equations was used to populate eight snapshot matrices (one for each unique set of equations). The previously described loading conditions were applied to each RUC. An SVD was performed on each snapshot matrix and was used to generate a set of orthonormal basis vectors. Figure 3 contains a plot of the first 30 singular values associated with each of the eight order-reduced models for the 256 subcell RUC (*i.e.*, Figure 2a). Similar plots were obtained for the other RUCs. Each of the models show a rapid decay in the magnitude of the singular values. This suggests that accurate order-reduced models can be likely be generated using a small number of basis vectors. Conceivably, each of the eight order-reduced HFGMC models for a given RUC can require a distinct number of basis vectors. Since the plot of the singular values was similar for the first six models (used to establish effective properties) and the boundary conditions are similar, a constant number of basis vectors was used for the first six models. Similarly, a different number of basis vectors was used for the remaining two models (used to solve the actual boundary value problem). Future studies will investigate more robust methods to establish the appropriate size of each order-reduced model within HFGMC.

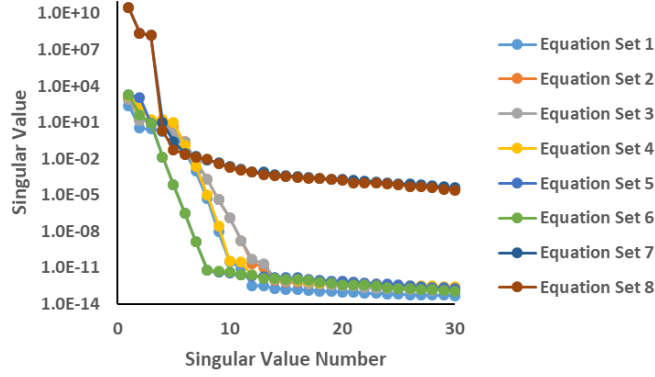


Figure 3. Singular values of the snapshot matrix for each set of simultaneous equations.

### Assessment of the Order-Reduced HFGMC Models for Determining Effective Properties

The accuracy of the order-reduced models was assessed by performing multiple simulations, each with a different number of basis vectors. Recall that the first six order-reduced models are used to establish RUC effective properties. Since these properties influence the global fields, the error in the effective elastic stiffness and thermal stress tensors was first determined by performing a series of analyses using one to ten basis vectors. Recall that for this study, the effective properties do not depend on inelastic state or applied mechanical loading and are only a function of temperature. Hence the temperature was varied over 150 increments consistent with the previous analyses and only the effective properties were determined at each temperature. The error at each increment (temperature) was calculated using the following relationship:

$$Err = \frac{\|A_R - A_{OR}\|_2}{\|A_R\|_2} \quad (8)$$

where  $A$  represents either the vectorized effective elastic stiffness tensor or the effective thermal stress tensor and the subscripts  $R$  and  $OR$  correspond to the reference or order-reduced vectors, respectively.  $\|\cdot\|_2$  denotes the  $L_2$ -norm. Figure 4 contains the error in the effective elastic stiffness tensor at each increment for multiple sizes of the order-reduced models. The error was observed to be relatively constant as the temperature varied for a given model. Furthermore, as the number of basis vectors used in the order-reduced models increased, the error steadily decreased. Similar trends were observed for the error in the effective thermal stress tensor. Since both the effective elastic stiffness and thermal stress tensors are calculated using the mechanical strain concentration tensor [1], the two tensors have similar errors for order-reduced models with the same number of basis vectors. Analogous error estimates in the effective properties for the remaining RUCs were obtained and closely resembled those of the 256 subcell RUC. Hence, for all RUCs,  $k = 5$  was determined to yield accurate effective properties and was used in subsequent assessments of the subcell/global fields. Effectively, the first six order-reduced models involved solving a dense set of  $k = 5$  equations while the reference model was comprised of a highly

sparse set of  $n = 1536-31,104$  equations depending on the RUC architecture considered.

### **Assessment of the Order-Reduced HFGMC Models for Determining Global/Local Fields**

In order to assess the accuracy of the remaining two order-reduced models for each RUC architecture, the global and subcell stress fields were evaluated for multiple order-reduced models where the size varied from  $k = 1-25$ . As previously mentioned, each of these two models used the same number of basis vectors for a given simulation. The error was calculated using Eq. 8 where  $A$  now represents the  $6 \times 1$  global or subcell stress vector. The average error in global stresses across all iterations for a given size order-reduced model are plotted in Figure 5. The error in subcell stresses was averaged across all iterations and subcells and is also shown. In general, as the size of the order-reduced models increased, the average error in both the global and subcell stresses decreased. Additionally, the average error in subcell stresses was typically greater than that of the global stresses. Minor differences in the order-reduced approximations are more likely to result in a greater error in the local, subcell stress fields rather than the global, homogenized stress field. This also suggests that, in general, a larger size order-reduced model is likely required to obtain more accurate subcell fields than global fields. However, for the RUCs considered in this study, a similar level of accuracy in global and subcell fields can be obtained for the same size order-reduced model. As the RUC complexity is increased, no clear trend in the error is obvious. For instance, 11 basis vectors are required to generate 99% accurate order-reduced models for the 1024 subcell RUC while 9 are required for a more complex, 5184 subcell RUC. Hence the optimal size of the order-reduced models is likely problem specific and driven by local features (*i.e.*, regions of intense inelasticity). Some local instabilities were also observed for the 5184 subcell RUC for smaller order-reduced models ( $k = 3,4$ ). In both cases, the model became unstable near the maximum applied load. This issue is currently being investigated.

The computational efficiency of the order-reduced models was assessed for each RUC architecture. Since it is computationally intensive to write individual subcell level information to data files, the efficiency of the reference and order-reduced models was determined by suppressing all subcell output and repeating the above analyses. The time spend assembling/solving the HFGMC systems of equations was determined for the reference model and the order-reduced models. Recall that the order-reduced model requires mapping to and from the order-reduced system of equations at each increment/iteration (*i.e.*, additional matrix multiplications are required). The computation runtimes for the order-reduced models include both the time needed to perform the mapping and solution of the equations. Speedup factors were calculated by dividing the reference solution runtime by the order-reduced runtime. The speedup factors calculated from the assembly/solution runtimes are shown in Figure 6 for order-reduced models with up to 15 basis vectors. In all of these simulations, the first six HFGMC systems of equations was of size ( $k = 5$ ) as previously mentioned. Regardless of the RUC, as the size of the order-reduced model increased, the speedup decreased as would be expected. However, relatively small order-reduced HFGMC models ( $10 < k < 25$ ) generally required *more* time to run than the reference model. For example, while the 1024 subcell RUC order-reduced models with 9 basis vectors gave less than a 1% error in stress fields, it required

approximately the same amount of time to run as the reference solution. However, for all of the RUCs, there was a small window where modest computational savings can be achieved at the expense of some accuracy. For instance, the order-reduced models ( $k = 6$ ) for the 2116 subcell RUC had a speedup factor of approximately 1.5 and yielded 99% accurate stresses. The lack of significant speedup in general is likely an artifact of the HFGMC solution process. For the reference model, the core computational effort involves assembling and factoring the stiffness matrix and is performed only once per increment (if a temperature change occurs). In the order-reduced models, the full stiffness matrix is assembled once per increment as well. However, the mapping operations required to generate the order-reduced systems of equations are performed eight separate times per increment. This repeated mapping underscores the need for more computationally efficient assembly/mapping algorithms (*e.g.*, direct assembly [11-12]) in order to further assess the usefulness of order-reduction techniques to HFGMC. Such techniques can allow the order-reduction to be applied on the subcell level (size  $k$ ) rather than continually mapping to and from the original global level (size  $n$ ) [12]. Ongoing work is focused on developing these procedures.

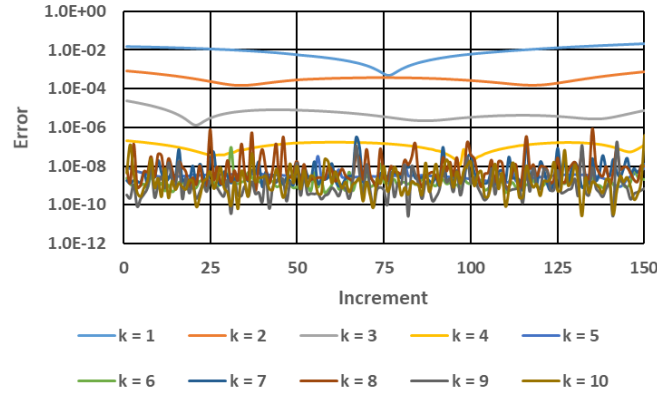


Figure 4. Error in the effective elastic stiffness tensor for the 256 subcell RUC at each increment for multiple order-reduced models.

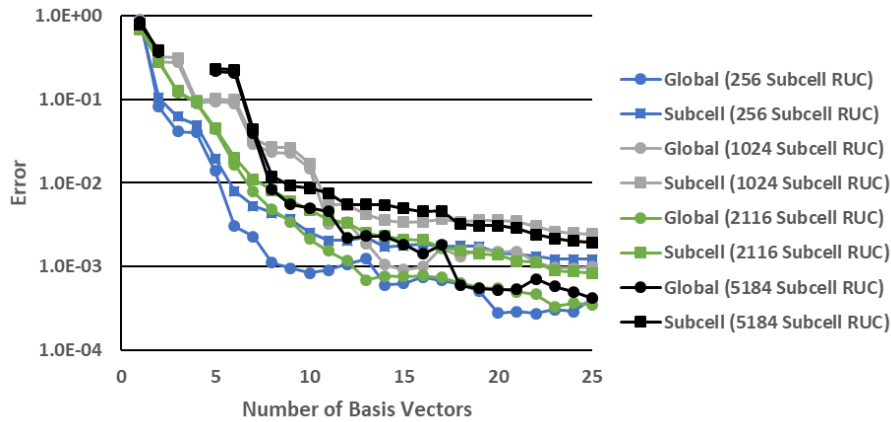


Figure 5. Average error in the global/subcell stresses for each RUC for multiple order-reduced models.

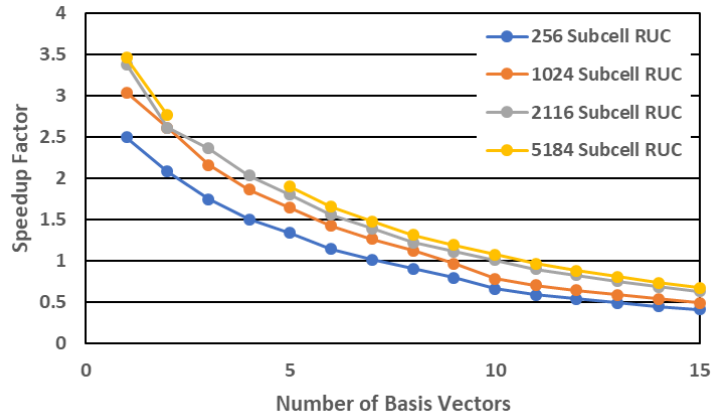


Figure 6. Speedup factors for each RUC as the order-reduced model size increases.

## CONCLUSIONS

In this study, the High-Fidelity Generalized Method of Cells (HFGMC) global system of  $n \times n$  equations for doubly-periodic repeating unit cells (RUCs) with thermoelastic constituents was reduced in size through the use of proper orthogonal decomposition with Petrov-Galerkin projection. The reduced  $k \times k$  system of equations ( $k \ll n$ ) was compared to the unmodified HFGMC equations for micromechanics models four distinct RUCs of increasing complexity (256 to 5184 subcells). For all RUCs, relatively small order-reduced models were found to accurately reproduce effective properties ( $k = 5$ ) and global/subcell stresses ( $k = 6-11$ ). A speedup of 1.2-1.5 in several RUCs was achieved while maintaining accuracy. However, the order-reduced models were not computationally feasible once the size exceeded  $k = 10$ . Current work is aimed at further improving the computational efficiency of the order-reduced HFGMC by performing order-reduction at the subcell level rather than the global level.

## ACKNOWLEDGEMENT

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## REFERENCES

1. Aboudi J., S. M. Arnold, and B. A. Bednarczyk. 2012. *Micromechanics of Composite Materials: A Generalized Multiscale Analysis Approach*. Butterworth-Heinemann.
2. Liang Y. C., H. P. Lee, S. P. Lim, W. Z. Lin, K. H. Lee, and C. G. Wu. 2002. "Proper Orthogonal Decomposition and Its Applications - Part I: Theory," *J. Sound Vib.*, 252(3):527-544.
3. Chatterjee A. 2000. "An Introduction to the Proper Orthogonal Decomposition," *Curr. Sci.*, 78(7):808-817.
4. Radermacher A., B. A. Bednarczyk, B. Stier, J. Simon, L. Zhou, and S. Reese. 2016. "Displacement-Based Multiscale Modeling of Fiber-Reinforced Composites by Means of Proper Orthogonal Decomposition," *Adv. Model. and Simul. in Eng. Sci.*, 3(29).
5. Radermacher A., S. Reese, and A. M. H. Hadoush. 2013. "Selective Proper Orthogonal Decomposition Model Reduction for Forming Simulations," *Proc. Appl. Math. Mech.*, 13:115-116.

6. Hernandez J. A., J. Oliver, A. E. Huespe, M. A. Caicedo, and J. C. Cante. 2014. "High-Performance Model Reduction Techniques in Computational Multiscale Homogenization," *Comput. Methods Appl. Eng.*, 276:149-189.
7. Yvonnet J. and Q.-C. He. 2007. "The Reduced Model Multiscale Method (R3m) for the Non-Linear Homogenization of Hyperelastic Media at Finite Strains," *J. Comput. Phys.*, 223:341-368.
8. Ricks T. M., J. Lacy, T.E., E. J. Pineda, B. A. Bednarczyk, and S. M. Arnold. 2016. "Computationally Efficient High-Fidelity Generalized Method of Cells Micromechanics Via Order-Reduction Techniques," *Compos. Struct.*, 156:2-9.
9. Bansal Y. and M.-J. Pindera. 2004. "Testing the Predictive Capability of the High-Fidelity Generalized Method of Cells Using an Efficient Reformulation," Report Number:NASA/CR-2004-213043.
10. Arnold S. M., B. A. Bednarczyk, and J. Aboudi. 2004. "Comparison of the Computational Efficiency of the Original Versus Reformulated High-Fidelity Generalized Method of Cells," Report Number:NASA/TM-2004-213438.11. Allen D. H. and W. E. Haisler. 1985. *Introduction to Aerospace Structural Analysis*. Wiley.
12. Radermacher A. 2014. *Proper Orthogonal Decomposition-Based Model Reduction in Nonlinear Solid Mechanics*. Rheinisch-Westfälischen Technischen Hochschule Aachen University.
13. Mendelson A. 1968. *Plasticity: Theory and Application*. Macmillan.
14. Bednarczyk B. A., J. Aboudi, and S. M. Arnold. 2006. "The Equivalence of the Radial Return and Mendelson Methods for Integrating the Classical Plasticity Equations," Report Number:NASA/TM-2006-214331.
15. Sirovich L. 1987. "Turbulence and the Dynamics of Coherent Structures Part I: Coherent Structures," *Q. Appl. Math.*, 45(3):561-571.
16. Carlberg K., C. Bou-Mosleh, and C. Farhat. 2011. "Efficient Non-Linear Model Reduction Via a Least-Squares Petrov–Galerkin Projection and Compressive Tensor Approximations," *Int. J. Numer. Meth. Engng.*, 86:155-181.
17. Kaddour A. S., M. J. Hinton, P. A. Smith, and S. Li. 2013. "Mechanical Properties and Details of Composite Laminates for the Test Cases Used in the Third World-Wide Failure Exercise," *J. Compos. Mat.*, 47(20-21):2427-2442.
18. Serban D. A., G. Weber, L. Marsavina, V. V. Silberschmidt, and W. Hufenbach. 2013. "Tensile Properties of Semi-Crystalline Thermoplastic Polymers: Effects of Temperature and Strain Rates " *Polym. Test.*, 32(2):413-425.
19. McNally T., W. R. Murphy, C. Y. Lew, R. J. Turner, and G. P. Brennan. 2003. "Polyamide-12 Layered Silicate Nanocomposites by Melt Blending," *Polym.*, 44(9):2761-2772.
20. Murthy P. and E. J. Pineda. 2016. "Tool for Generation of Mac/Gmc Representative Unit Cell for Cmc/Pmc Analysis," Report Number:NASA/TM-2016-219127.